

Supporting Information

Convergent Mechanistic Features between the Structurally Diverse N- and O-Methyltransferases: Glycine N-Methyltransferase and Catechol O-Methyltransferase

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Scheme S1 Conversion between open and closed conformations for dimer structures of rat GNMT in the presence of AdoMet and acetate.¹ Residues 1-23 are shown in blue and red in each subunit (cyan and yellow) illustrated in cartoon. AdoMet and acetate are presented in sticks with C(green), N(blue), O(red) and S(yellow). (a) apo-GNMT, open and inactive conformation, PDB:1BHJ;² (b) Binary complex with R175K GNMT and AdoMet, the residue 1-17 is not shown for the immobile position in crystal structure. PDB:1NBI; (c) Ternary complex with GNMT, AdoMet and acetate. PDB:1NBH.

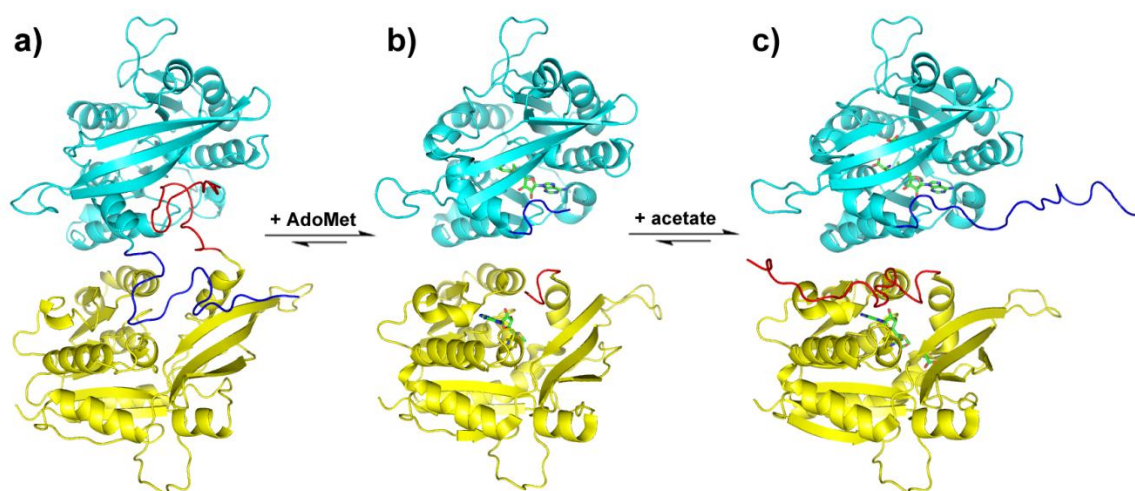


Figure S1 Relationship between the k_{cat}/K_m for AdoMet and 2° KIE for methylation of Glycine by the Recombinant Rat GNMT and Y21 mutants.

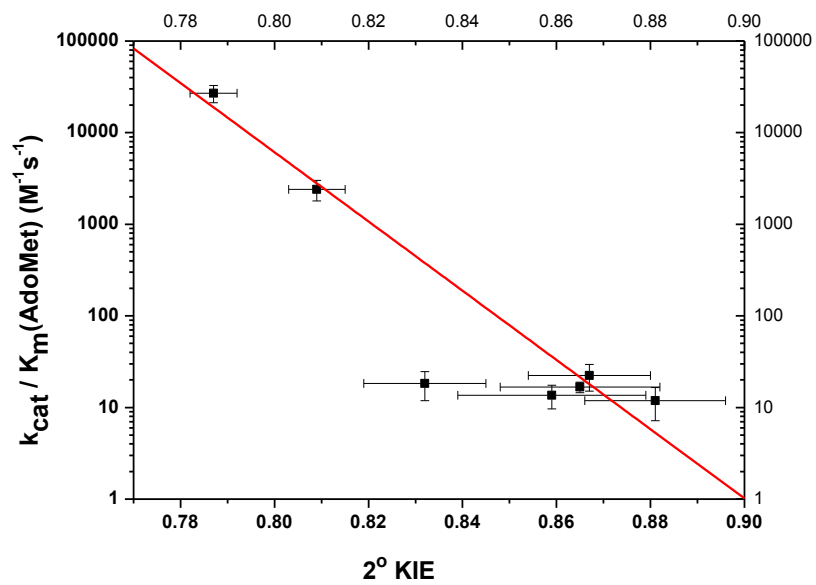


Figure S2 Using the ternary complex of GNMT with acetate as a model, the carboxylate group of substrate is expected to be anchored by hydrogen bond interactions with Tyr33, Asn138, Arg175 and Tyr220.

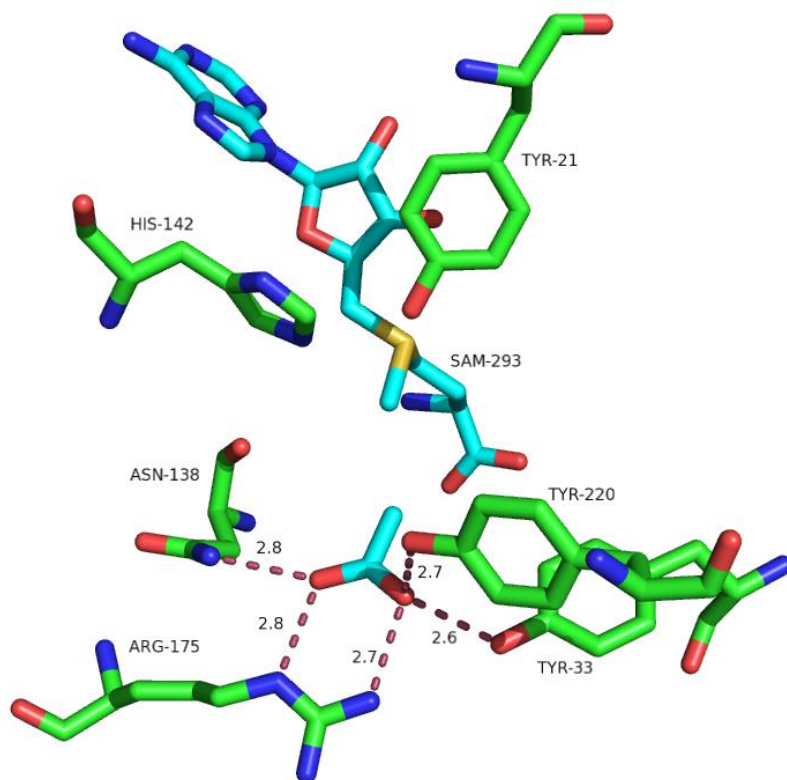


Fig S3 Schematic diagram showing the interaction of glycine (in green) in the active site of GNMT (PDB: 1NBH with glycine docking in the active site).

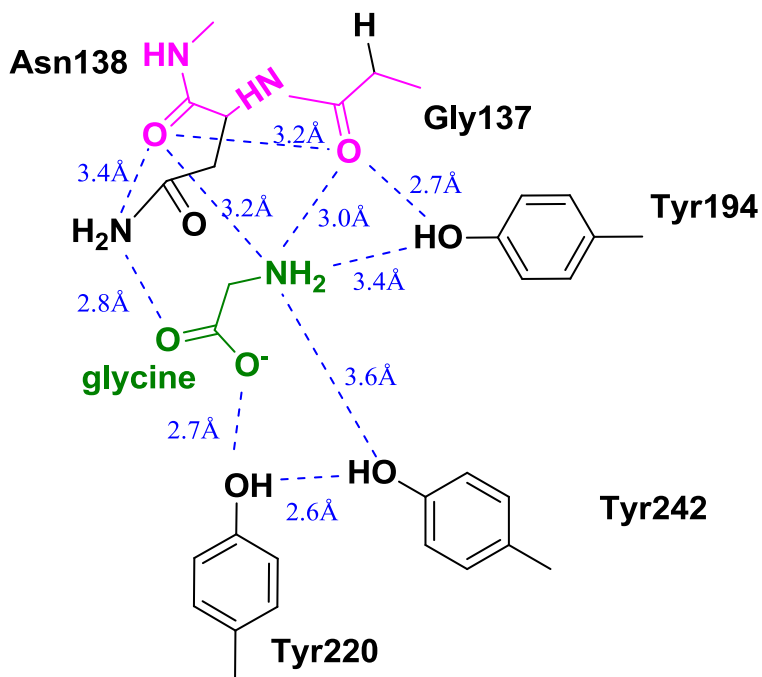
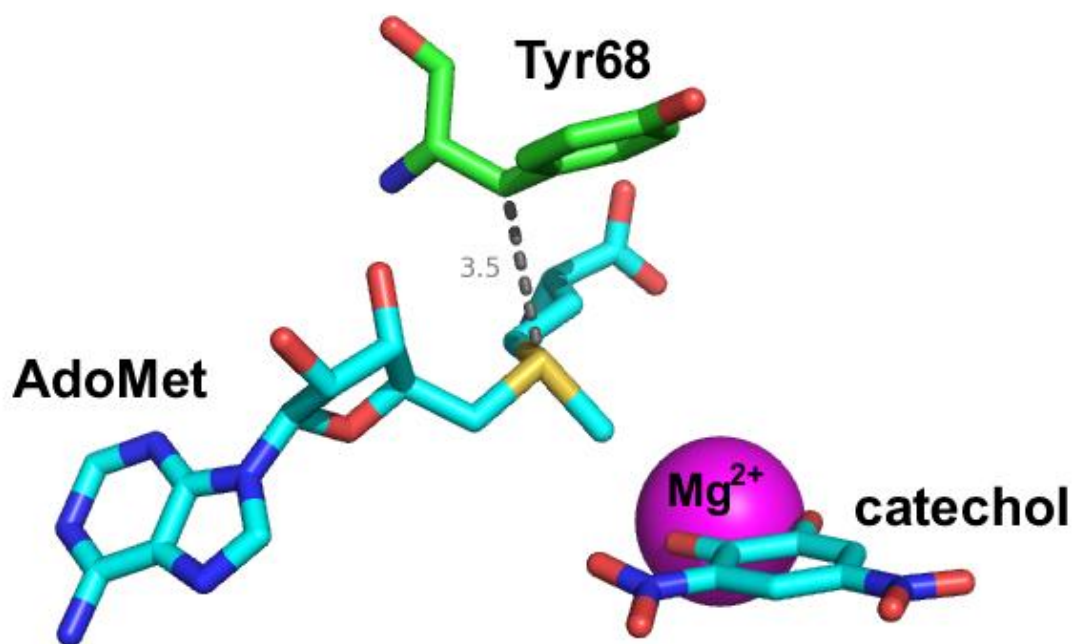


Fig S4 Active site of COMT.



References:

- (1) Takata, Y.; Huang, Y. F.; Komoto, J.; Yamada, T.; Konishi, K.; Ogawa, H.; Gomi, T.; Fujioka, M.; Takusagawa, F. *Biochemistry* **2003**, *42*, 8394.
- (2) Pattanayek, R.; Newcomer, M. E.; Wagner, C. *Protein Science* **1998**, *7*, 1326.